

Magnetic phase diagrams of the generalized spin-one-half Falicov-Kimball model

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Abstract

A combination of small-cluster exact-diagonalization calculations and a well-controlled approximative method is used to examine the ground-state phase diagrams of the spin-one-half Falicov-Kimball model extended by the spin-dependent on-site interaction (J) between localized spins and itinerant (d) electrons, as well as by external magnetic field (h). Both the magnetic ordering and metamagnetic transitions are analysed as functions of h and the number of itinerant electrons (N_d) at selected J . Various magnetic superstructures including axial and diagonal spin stripes are observed for nonzero values of J and h . Moreover, it is shown that increasing h strongly stabilizes the fully and partially polarized states, while the non polarized state is reduced.

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1 Introduction

In the past decade, a considerable amount of effort has been devoted to understand the underlying physics that leads to a charge ordering in strongly correlated electron systems. The motivation was clearly due to the observation of a such ordering in doped nickelate [1] and cuprate [2] materials, some of which constitute materials that exhibit high-temperature superconductivity. One of the simplest models suitable to describe charge ordered phases in interacting electron systems is the Falicov-Kimball model (FKM) [3]. Indeed, it was shown that already the simplest version of this model (the spinless FKM) exhibits an extremely rich spectrum of charge ordered solutions, including various types of periodic, phase-separated and striped phases [4, 5]. However, the spinless version of the FKM, although non-trivial, is not able to account for all aspects of real experiments. For example, many experiments show that a charge superstructure is accompanied by a magnetic superstructure [1, 2]. In order to describe both types of ordering in the unified picture, it was proposed [6] a simple model based on a generalization of the spin-one-half FKM with an anisotropic, spin-dependent local interaction that couples the localized and itinerant subsystems. The first systematic studies [6, 7] clearly demonstrated strong cooperative effects of spin-dependent interaction on the ground states of the model and revealed various types of homogeneous as well as inhomogeneous ordering. It is naturally to expect, that the formation of new structures is accompanied by changes in magnetization, and therefore we would like to study the ground-state properties of the model in the external magnetic field. The motivation for our study was also the work by Lemański [8], where similar studies were performed using the restricted phase diagram method for 12 periodic configurations of the spins. Here we study the model exactly (over the full set of spin configurations) for clusters up to 36 lattice sites and approximately for larger clusters.

Our starting Hamiltonian has the form

$$\begin{aligned}
 H = \sum_{ij\sigma} t_{ij} d_{i\sigma}^+ d_{j\sigma} &+ J \sum_i (d_{i\uparrow}^+ d_{i\uparrow} - d_{i\downarrow}^+ d_{i\downarrow}) S_i^z \\
 &- h \sum_i (d_{i\uparrow}^+ d_{i\uparrow} - d_{i\downarrow}^+ d_{i\downarrow}) - h \sum_i S_i^z,
 \end{aligned} \tag{1}$$

where S_i^z is a spin projection in z direction with values $S_i^z = \pm 1$, and $d_{i\sigma}^+$, $d_{i\sigma}$ are the creation and annihilation operators of the itinerant electrons in the d -band Wannier state at site i .

The first term of (1) is the kinetic energy corresponding to quantum-mechanical hopping of the itinerant d -electrons between sites i and j . These intersite hopping transitions are described by the matrix elements t_{ij} , which are $-t$ if i and j are the nearest neighbors and zero otherwise (in the following all parameters are measured in units of t). The second term is anisotropic, spin-dependent local interaction of the Ising type between the d -electrons and spins. The last two terms represent energies of d -electrons and spins in an external magnetic field.

Using the fact, that S_i^z takes only two values $S_i^z = \pm 1$ the Hamiltonian (1) can be rewritten as

$$H = \sum_{ij\sigma} t_{ij}^\sigma d_{i\sigma}^+ d_{j\sigma} - h \sum_i S_i^z, \quad (2)$$

where $t_{ij}^\sigma = t_{ij} + \sigma(J S_i^z - h)\delta_{ij}$. Thus for a given spin distribution $s = \{S_1^z, S_2^z, \dots, S_L^z\}$, the Hamiltonian (2) is the second-quantized version of the single particle Hamiltonian $t^\sigma(s)$, so the investigation of the model (2) is reduced to the investigation of the spectrum of t^σ for different configurations of spins. This can be done exactly over the full set of spin configurations or approximately over a reduced set. In this paper we present a combination of both methods. For clusters up to $L = 36$ lattice sites we use small-cluster exact-diagonalization calculations and for larger clusters we use the well-controlled numerical method described in detail in the papers [9].

2 Results and discussion

In the present work we study the one ($D = 1$) and two ($D = 2$) dimensional analogue of the model for the spin interaction value $J = 0.5$ and for a wide range of magnetic field h (from $h = 0$ to $h = 0.5$ with step 0.01). To reveal the finite-size effects numerical calculations were done on different clusters. We have found, that the main features of the phase diagrams in the $N_d - h$ plane (for $D = 1$ as well as $D = 2$) hold on all examined lattices and thus can be used satisfactorily to represent the behaviour of macroscopic systems. Here we present the one dimensional results for $L = 24$, that represent the typical one-dimensional behaviour, while for $D = 2$ the

numerical results are presented for $L = 36$ (the largest cluster that we were able to consider exactly).

Let us start a discussion of the phase diagram with a description of configuration types that form its basic structure in one dimension. Manifold phases entered into the phase diagrams are classified according to $S^z = \sum_i S_{i\uparrow}^z - S_{i\downarrow}^z$ and $S_d^z = N_{d\uparrow} - N_{d\downarrow}$: the fully polarized (FP) phase characterized by $|S^z| = L$, $|S_d^z| = N_d$, the partially polarized (PP) phases characterized by $0 < |S^z| < L$, $0 < |S_d^z| < N_d$ and the non polarized (NP) phases characterized by $|S^z| = 0$, $|S_d^z| = 0$. Comparing these phase diagrams with ones obtained for $h = 0$ [7], one can see rather different behaviours. Indeed, while for $h = 0$ the magnetic phase diagrams coincide practically over the whole range of model parameters, the non-zero h destroys obviously this coincidence. Now the phase diagrams coincide only at low d -electron concentrations where the ground state is the FP phase for both the d -electron as well as spin subsystems. But with increasing N_d the spin and d -electron systems are developed differently. For higher values of N_d the spin subsystem still prefers the FP state, contrary to the d -electron subsystem where the PP state is stabilized. A different behaviour is observed also for $h \rightarrow 0$, where the spin subsystem prefers PP state, while the d -electron subsystem prefers the NP state. Besides these differences the phase diagrams of spin and d -electron subsystems exhibit one same characteristic and namely that very small changes of h can produce large cooperative changes, indicating possible metamagnetic transitions. Before discussing these transitions let us discuss the complete set of ground state configurations, that enter to the spin phase diagram. The complete set of ground-state configurations consists of only a few types, including 7 different NP phases, 10 different PP phases and of course the FP phase. Between them one can find different types of periodic or perturbed periodic and non-periodic configurations, but the most interesting examples represent NP phases. In this case all configurations (with the exception of $N_d = 22$) have a central point symmetry.

Let us now turn on our attention to the problem of metamagnetic transitions. To reveal the structure of magnetization curves we have performed exhaustive studies of the model for two different d -electron concentrations $n_d = 1/2$ and $n_d = 3/4$. In Fig. 2 we summarize numerical results for both electron as well as spin subsystems. In the first case ($n_d = 1/2$) the spin magnetization curve consists of two significant

stairs (see Fig. 2a) $m_f = 0$ and $m_f = 1$ (or $m_d = 0$ and $m_d \sim 0.5$ for d -electrons, see Fig. 2b). It is very interesting, that the relative small changes of h lead to the significant spin reorientation from the periodic arrangement $\{\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow \dots \downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\}$ ($m_f = 0$) to the FP state ($m_f = 1$). The similar situation holds also for $n_d = 3/4$, where the transition from the NP phase to the FP phase realizes through the PP states (Fig. 2c). In the spin magnetization curve we have observed four significant stairs ($m_f = 0, 1/4, 1/3$ and 1) corresponding to four different configuration types ($w_0 = [\uparrow\uparrow\downarrow\downarrow\uparrow\downarrow]_{L/8}, w_{1/4} = [\uparrow\uparrow\downarrow\uparrow\uparrow\downarrow\downarrow]_{L/8}, w_{1/3} = [\uparrow\uparrow\downarrow]_{L/3}$ and $w_1 = \{\uparrow \dots \uparrow\}$, where the lower index denotes the number of repetitions of the block [...]). The same structure is observed also on the d -electron magnetization curve as illustrates Fig. 2d.

Let us now briefly discuss the case $D = 2$. In Fig. 3 we present the phase diagrams of the model in the $N_d - h$ plane obtained by exact-diagonalization calculations for $L = 36$ and $J = 0.5$. Comparing these phase diagrams with their one-dimensional counterparts one can find obvious similarities. Again the phase diagrams coincide only at very low d -electron concentrations where the ground state is the FP phase, while for increasing N_d the spin (d -electron) subsystem prefers the FP (PP) state. The NP ground states for non-zero h are observed only on isolated lines (points) at N_d : $N_d = 18, 26$ for spins and $N_d = 2, 10, 18, 26$ and 36 for d -electrons.

The two-dimensional results are of particular importance since they could shed light on the mechanism of two-dimensional charge and magnetic ordering in doped nickelate [1] and cuprate [2] materials. Here we concern our attention on a description of basic types of magnetic ordering that exhibits the spin-one-half FKM with spin-dependent interaction between d -electrons and spins in the magnetic field h for $D = 2$. Analysing obtained numerical data, it was found that the set of ground-state configurations consists of only a few basic configuration types, listed in Fig. 4.

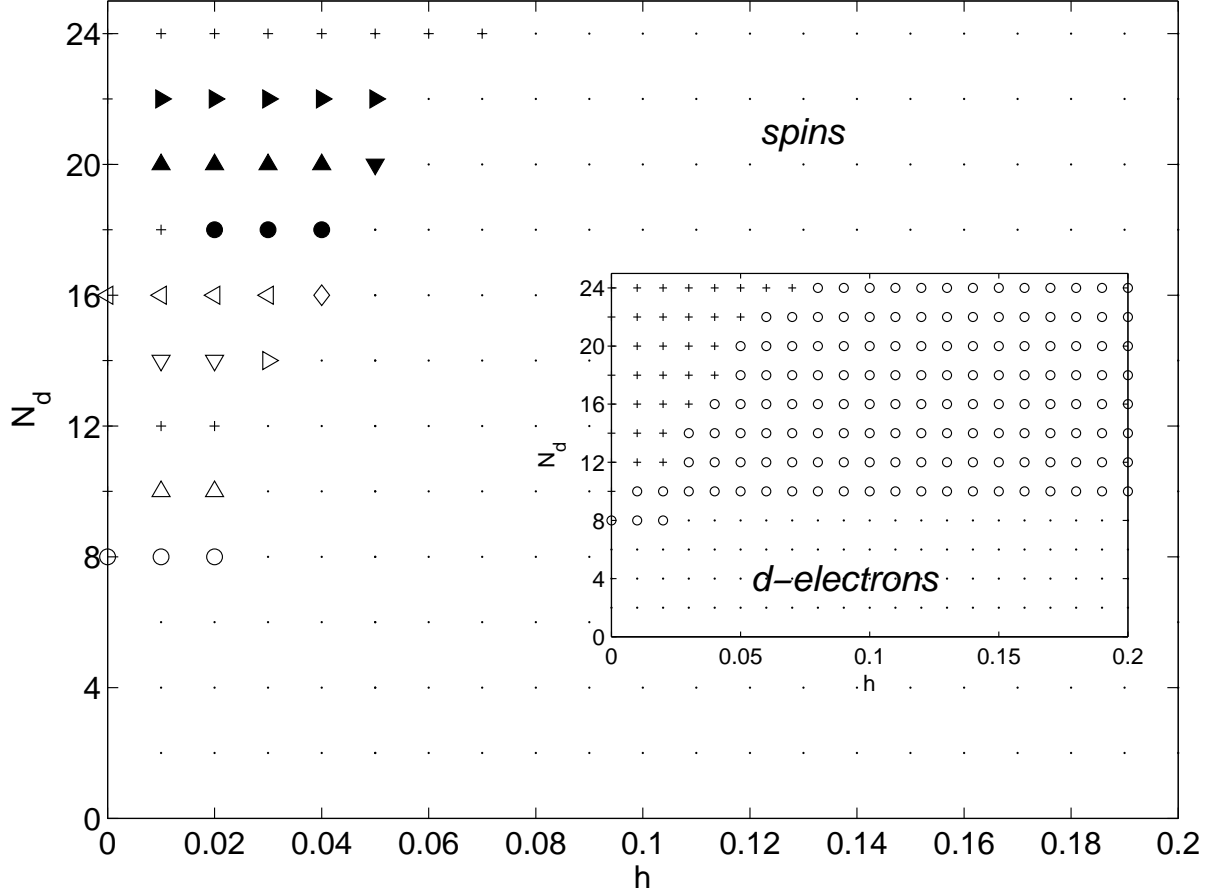
With increasing N_d one can see a general tendency of the system to change the ground state from the phase separation (observed for small N_d) through special inhomogeneous axial stripes (intermediate N_d) to the regular "chessboard" structure (around $N_d = L$). Moreover, the unusual central point symmetry observed for NP phases in $D = 1$ case persists also for $D = 2$ (for all NP states with the exception of $N_d = 10$ and $N_d = 22$), of course now as a mirror symmetry. Again, we have studied the magnetizations for spin as well as d -electron subsystems on clusters up to

$L = 100$ lattice sites. Unfortunately, we were not able to obtain the definite results, due to finite-site effects.

In summary, a combination of small-cluster exact diagonalization calculations and a well-controlled approximative method was used to study the ground-state phase diagrams of the generalized spin-one-half FKM with spin-dependent on-site interaction $J = 0.5$ extended by magnetic field for one and two dimensional cases. For both cases it was found that the magnetic field stabilizes the FP (for spins) or PP/FP states (for d -electrons), while the NP states persist only for $h \rightarrow 0$. Although, the non-zero h destroys the coincidence between the spin and d -electron subsystems (observed for $h = 0$), the one common feature is evident, and namely, that the very small changes of h can produce large cooperative changes in the ground state of the model. This observation was supported also by studies of magnetization curves, where we have observed strong changes from the periodic NP/PP state to the FP state as well as with configuration type analysis, where we have identified phase separated, striped, periodic and non-periodic spin distributions.

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Partially polarized phases:

- $\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow$
- △ $\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow$
- ▽ $\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow$
- ▷ $\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow\uparrow\uparrow\uparrow\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow$
- ◁ $\uparrow\uparrow\uparrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\uparrow\downarrow\uparrow\downarrow\uparrow\uparrow\downarrow\uparrow\downarrow\uparrow\uparrow$
- ◇ $\uparrow\uparrow\uparrow\uparrow\downarrow\uparrow\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow$
- $\uparrow\uparrow\downarrow\uparrow\uparrow\downarrow\uparrow\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow\downarrow$
- ▲ $\uparrow\uparrow\downarrow\uparrow\uparrow\downarrow\uparrow\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow\downarrow$
- ▼ $\uparrow\uparrow\uparrow\uparrow\downarrow\uparrow\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow\uparrow\uparrow\downarrow\uparrow\downarrow\uparrow\uparrow\uparrow$
- $\uparrow\uparrow\downarrow\uparrow\uparrow\downarrow\uparrow\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow\downarrow\uparrow\uparrow\downarrow$

Non polarized phases:

- + ($N_d=10$) $\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow$
- + ($N_d=12$) $\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow$
- + ($N_d=14$) $\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow\uparrow\uparrow\downarrow\downarrow$
- + ($N_d=18$) $\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow$
- + ($N_d=20$) $\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow$
- + ($N_d=22$) $\uparrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow$
- + ($N_d=24$) $\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow\uparrow\downarrow$

Fully polarized phase:

- \uparrow

Figure 1: Spin phase diagram of the model for $J = 0.5$ in the $N_d - h$ plane for $L = 24$ and $D = 1$. Inset: Magnetic phase diagram of the d -electron subsystem. Different symbols represent different magnetic phases: FP (·), PP (○) and NP (+) phases.

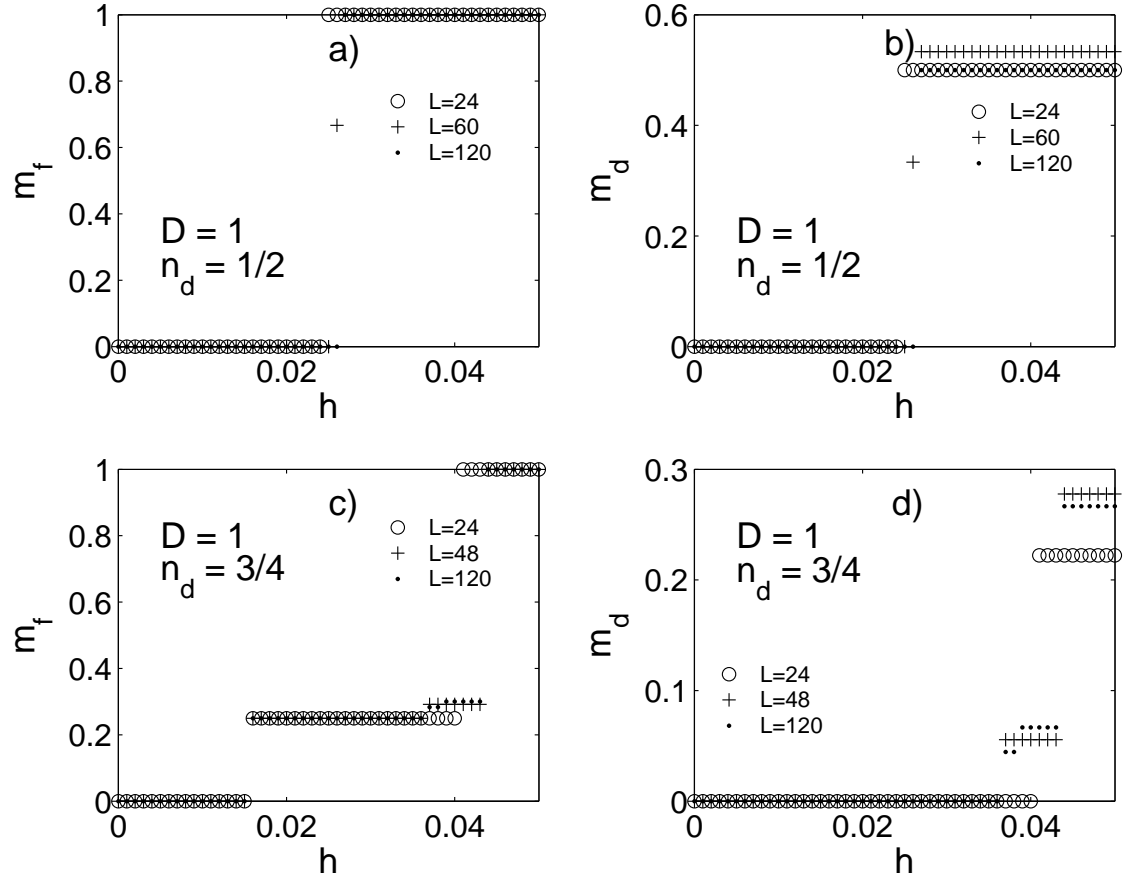


Figure 2: a) The total magnetization of the spins for $J = 0.5$, $n_d = 1/2$ and different clusters ($L = 24, 60$ and 120) in $D = 1$. b) Magnetization of electrons for the same parameters. c) The total magnetization of the spins for $J = 0.5$, $n_d = 3/4$ and different clusters ($L = 24, 48$ and 120) in $D = 1$. d) Magnetization of electrons for the same parameters.

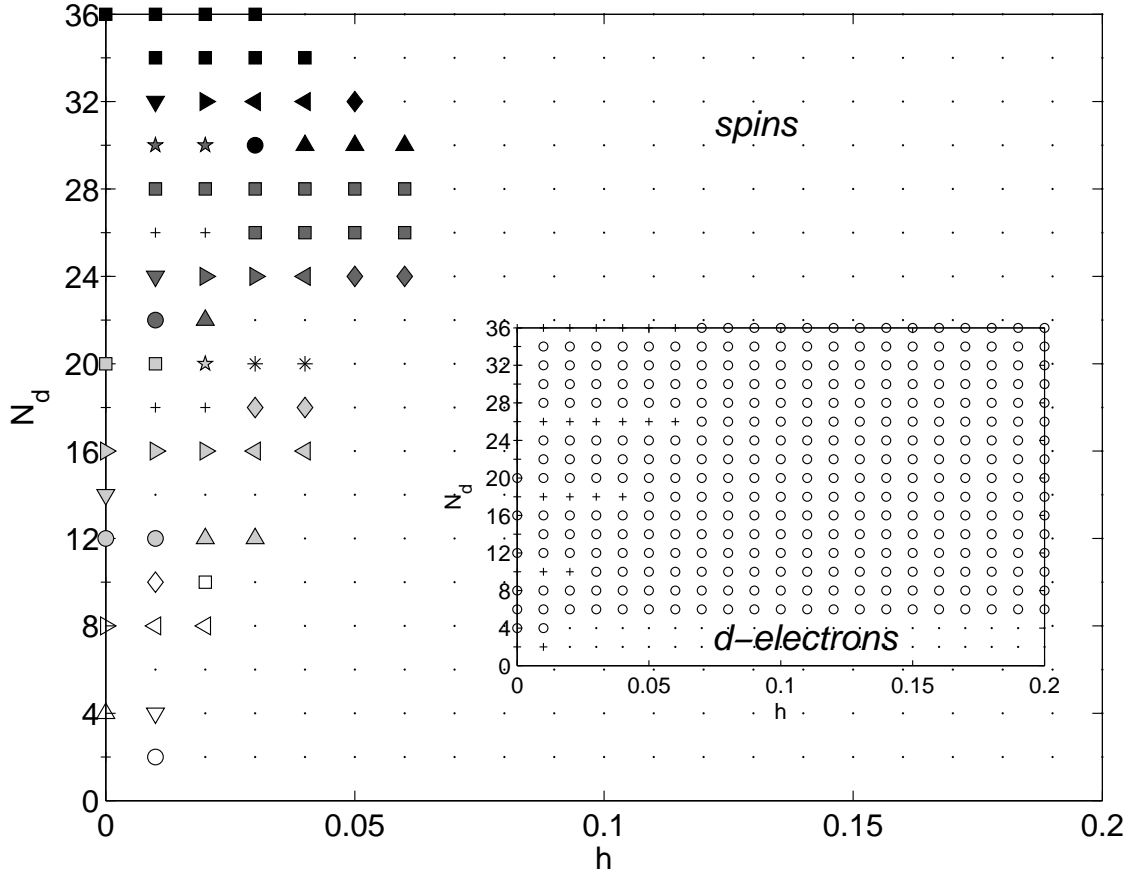


Figure 3: Spin phase diagram of the model for $J = 0.5$ in $N_d - h$ plane for $L = 36$ and $D = 2$. All ground-state configurations (with the exception of FP (.)) are displayed in Fig. 4. Inset: Magnetic phase diagram of the d -electron subsystem. Different symbols represent different magnetic phases: FP (.), PP (o) and NP (+) phases.

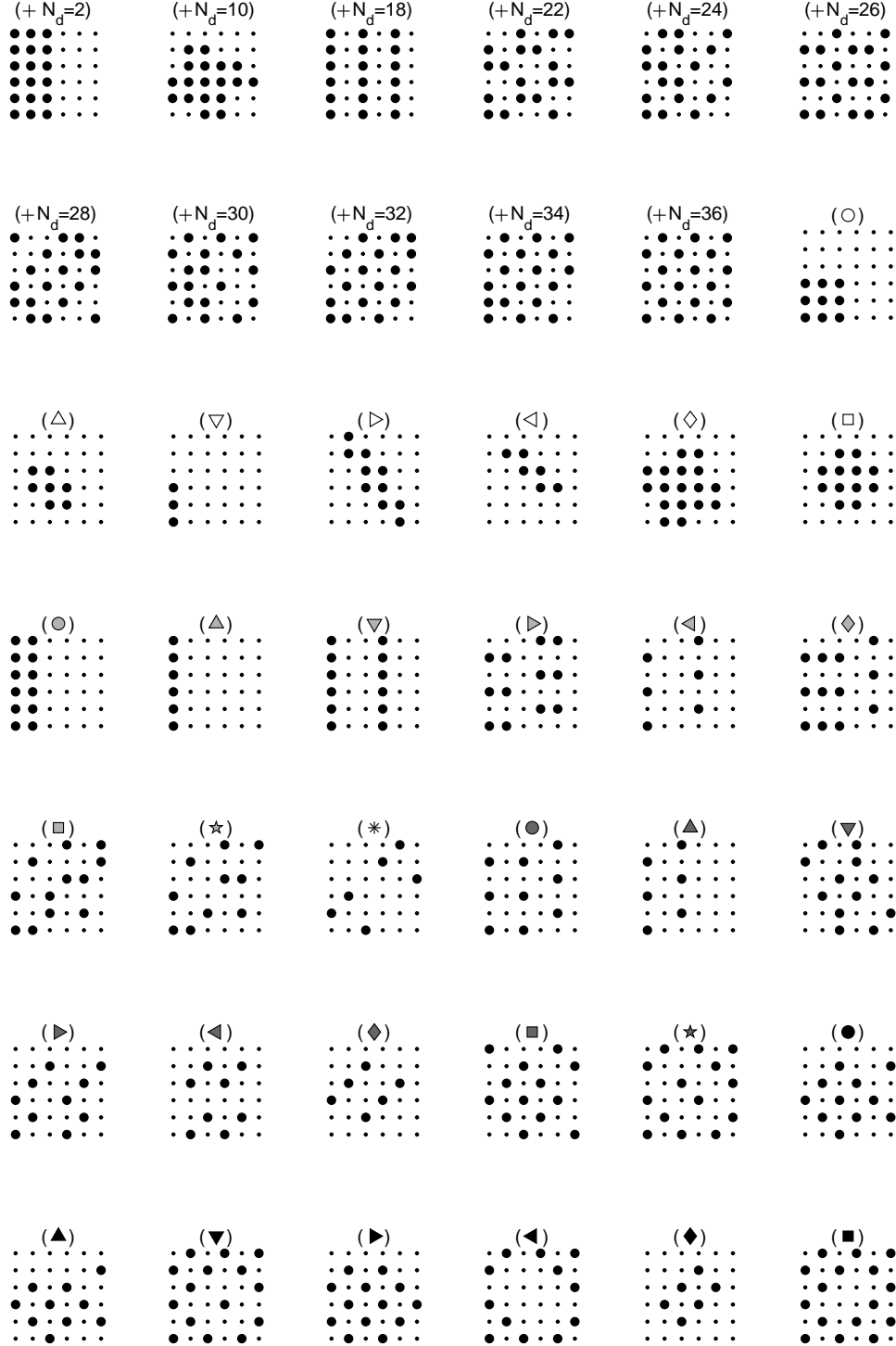


Figure 4: Arrangements of localized spins that enter into the phase diagram displayed in Fig. 3. First 11 phases correspond with NP phases. All other phases are PP. To visualize the spin distributions we use (\bullet) for the up spin orientation and (\cdot) for the down spin orientation.